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COMMENT ON "CALCULATION OF THE QUARKONIUM SPECTRUM AND m_b, m_c TO ORDER α_s^4"

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Abstract

A recent determination of the mass of the b quark, based exclusively on quantum chromodynamics (by avoiding strictly to introduce any phenomenological interaction potential of nonperturbative origin), may be improved by allowing for a merely numerical solution of the corresponding eigenvalue problem.

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Recently, Pineda and Ynduráin [1] presented a re-analysis of heavy quarkonia. Their investigation is based on the main assumption that bound systems of heavy quarks may be reasonably described by nonrelativistic kinematics and only the perturbative contribution to the quark–antiquark interaction potential V if all nonperturbative effects are taken into account by some appropriate correction to the energy. In order to describe a system of a heavy quark and antiquark, both with constituent mass m, forming a bound state with total spin $s = 0$ or $s = 1$, Pineda and Ynduráin consider the Hamiltonian

$$\begin{aligned} H &= 2\,m - \frac{1}{m}\,\Delta - \frac{1}{4\,m^3}\,\Delta^2 + V_0^{\rm P}(r) + \frac{C_{\rm F}\,\alpha(\mu)}{m^2\,r}\,\Delta + \frac{C_{\rm F}\,\alpha^2(\mu)}{4\,m\,r^2}\,(C_{\rm F} - 2\,C_{\rm A}) \\ &+ \frac{4\,\pi\,C_{\rm F}\,\alpha(\mu)}{3\,m^2}\,s\,(s+1)\,\delta^{(3)}({\bf x})\;, \quad r \equiv |{\bf x}|\;. \end{aligned} \tag{1}$$

The perturbative contribution to the static quark–antiquark interaction potential, $V_0^{\rm P}(r)$, is known up to and including the two-loop level [2]:

$$\begin{aligned} V_0^{\rm P}(r) &= -C_{\rm F}\,\frac{\alpha(\mu)}{r}\left\{1 + \frac{\alpha(\mu)}{4\,\pi}\left[\frac{5}{3}\,\beta_0 - \frac{8}{3}\,C_{\rm A} + 2\,\beta_0\,[\ln(\mu\,r) + \gamma_{\rm E}]\right]\right. \\ &+ \left(\frac{\alpha(\mu)}{4\,\pi}\right)^2\left[\beta_0^2\left(4\,[\ln(\mu\,r) + \gamma_{\rm E}]^2 + \frac{\pi^2}{3}\right) + \left(2\,\beta_1 + \frac{20}{3}\,\beta_0^2 - \frac{32}{3}\,\beta_0\,C_{\rm A}\right)[\ln(\mu\,r) + \gamma_{\rm E}]\right. \\ &+ \left(\frac{4343}{162} + 4\,\pi^2 - \frac{\pi^4}{4} + \frac{22}{3}\,\zeta(3)\right)C_{\rm A}^2 - \left(\frac{1798}{81} + \frac{56}{3}\,\zeta(3)\right)n_{\rm f}\,C_{\rm A}\,T_{\rm F} \\ &\left.\left. - \left(\frac{55}{3} - 16\,\zeta(3)\right)n_{\rm f}\,C_{\rm F}\,T_{\rm F} + \frac{400}{81}\,n_{\rm f}^2\,T_{\rm F}^2\right]\right\}. \end{aligned}$$

Here, the following notations have been adopted: $\alpha(\mu)$ denotes the strong fine-structure constant in the modified minimal-subtraction ($\overline{\rm MS}$) renormalization scheme. For a non-Abelian gauge theory for $n_{\rm f}$ Dirac fermions, invariant w. r. t. gauge transformations forming a Lie group SU(N) describing N colour degrees of freedom, the quadratic Casimir invariants read, for the fundamental representation,

$$C_{\rm F} = \frac{N^2 - 1}{2\,N}$$

and, for the adjoint representation,

$$C_{\rm A} = N\;,$$

if the generators of the Lie group SU(N) are normalized such that the second-order Dynkin index of the fundamental representation is

$$T_{\rm F} = \frac{1}{2}\;.$$

The dependence of the effective (running) fine-structure constant $\alpha(\mu)$ on the renormalization scale μ is described in terms of the Gell-Mann–Low β function according to

$$\frac{\mu}{2}\,\frac{\partial}{\partial\mu}\alpha(\mu) = -\frac{\alpha^2(\mu)}{4\,\pi}\,\beta_0 - \frac{\alpha^3(\mu)}{(4\,\pi)^2}\,\beta_1 - \frac{\alpha^4(\mu)}{(4\,\pi)^3}\,\beta_2 + O(\alpha^5)\;,$$

involving the well-known expressions for the (gauge-invariant) one-, two-, and three-loop expansion coefficients in the $\overline{\rm MS}$ scheme [3]

$$\begin{aligned} \beta_0 &= \frac{11}{3}\,C_{\rm A} - \frac{4}{3}\,n_{\rm f}\,T_{\rm F}\;, \\ \beta_1 &= \frac{34}{3}\,C_{\rm A}^2 - \frac{20}{3}\,n_{\rm f}\,C_{\rm A}\,T_{\rm F} - 4\,n_{\rm f}\,C_{\rm F}\,T_{\rm F}\;, \\ \beta_2 &= \frac{2857}{54}\,C_{\rm A}^3 - \frac{1415}{27}\,n_{\rm f}\,C_{\rm A}^2\,T_{\rm F} + \frac{158}{27}\,n_{\rm f}^2\,C_{\rm A}\,T_{\rm F}^2 - \frac{205}{9}\,n_{\rm f}\,C_{\rm A}\,C_{\rm F}\,T_{\rm F} + \frac{44}{9}\,n_{\rm f}^2\,C_{\rm F}\,T_{\rm F}^2 + 2\,n_{\rm f}\,C_{\rm F}^2\,T_{\rm F}\;. \end{aligned}$$

The resulting dependence of the fine-structure constant $\alpha(\mu)$ on the chosen renormalization scale μ, expressed in terms of the (standard) scale parameter Λ, reads up to and including the three-loop level

$$\begin{aligned} \alpha(\mu) &= \frac{4\,\pi}{\beta_0\ln(\mu^2/\Lambda^2)}\left\{1 - \frac{\beta_1}{\beta_0^2}\,\frac{\ln(\ln(\mu^2/\Lambda^2))}{\ln(\mu^2/\Lambda^2)}\right. \\ &+ \left.\frac{\beta_1^2}{\beta_0^4\ln^2(\mu^2/\Lambda^2)}\left[\left(\ln(\ln(\mu^2/\Lambda^2)) - \frac{1}{2}\right)^2 + \frac{\beta_2\,\beta_0}{\beta_1^2} - \frac{5}{4}\right]\right\}. \end{aligned}$$

$\gamma_{\rm E}$ is known as Euler–Mascheroni constant. In the case of quantum chromodynamics, clearly, $N = 3$.

Now, in order to stick to an entirely analytical analysis and following the philosophy developed in an earlier treatment [4] of heavy quarkonia, in Ref. [1] the static potential $V_0^{\mathrm{P}}(r)$ is split, according to

$$V_0^{\mathrm{P}}(r) = \tilde{V}(r) + \hat{V}(r) \ , \tag{2}$$

into the Coulomb-like contribution

$$\tilde{V}(r) \equiv -C_{\mathrm{F}} \, \frac{\tilde{\alpha}(\mu)}{r} \ ,$$

with the effective fine-structure constant

$$\begin{aligned}
\tilde{\alpha}(\mu) \ &\equiv \ \alpha(\mu) \left\{ 1 + \frac{\alpha(\mu)}{4\,\pi} \left(\frac{5}{3}\,\beta_0 - \frac{8}{3}\,C_{\mathrm{A}} + 2\,\beta_0\,\gamma_{\mathrm{E}} \right) \right. \\
&+ \ \left(\frac{\alpha(\mu)}{4\,\pi} \right)^2 \left[\beta_0^2 \left(4\,\gamma_{\mathrm{E}}^2 + \frac{\pi^2}{3} \right) + \left(2\,\beta_1 + \frac{20}{3}\,\beta_0^2 - \frac{32}{3}\,\beta_0\,C_{\mathrm{A}} \right) \gamma_{\mathrm{E}} \right. \\
&+ \ \left(\frac{4343}{162} + 4\,\pi^2 - \frac{\pi^4}{4} + \frac{22}{3}\,\zeta(3) \right) C_{\mathrm{A}}^2 - \left(\frac{1798}{81} + \frac{56}{3}\,\zeta(3) \right) n_{\mathrm{f}}\,C_{\mathrm{A}}\,T_{\mathrm{F}} \\
&- \ \left. \left. \left(\frac{55}{3} - 16\,\zeta(3) \right) n_{\mathrm{f}}\,C_{\mathrm{F}}\,T_{\mathrm{F}} + \frac{400}{81}\,n_{\mathrm{f}}^2\,T_{\mathrm{F}}^2 \right] \right\} ,
\end{aligned}$$

and an obvious remainder involving logarithms of the radial coordinate r,

$$\begin{aligned}
\hat{V}(r) \ &= \ -C_{\mathrm{F}} \, \frac{\alpha^2(\mu)}{4\,\pi\,r} \left\{ 2\,\beta_0 \, \ln(\mu\,r) \right. \\
&+ \ \left. \frac{\alpha(\mu)}{4\,\pi} \left[4\,\beta_0^2 \, \ln^2(\mu\,r) + \left(2\,\beta_1 + \frac{20}{3}\,\beta_0^2 - \frac{32}{3}\,\beta_0\,C_{\mathrm{A}} + 8\,\beta_0^2\,\gamma_{\mathrm{E}} \right) \ln(\mu\,r) \right] \right\} .
\end{aligned}$$

The eigenvalue problem for the Coulombic Hamiltonian

$$\tilde{H} \equiv 2\,m - \frac{1}{m}\,\Delta + \tilde{V}(r)$$

is solved exactly, yielding, for instance, for the ground state, the energy eigenvalue $\tilde{E}_0 = 2\,m + \varepsilon_0$, with the Coulomb binding energy

$$\varepsilon_0 = -\frac{C_{\mathrm{F}}^2\,\tilde{\alpha}^2(\mu)\,m}{4} \ .$$

The "non-Coulombic" part $H - \tilde{H}$ of the Hamiltonian (1) is treated perturbatively. Counting carefully the powers of α yields analytical expressions for the eigenvalues of H correct up to and including the order α^4. Nonperturbative effects are incorporated by adding the Leutwyler–Voloshin correction [5], which involves the gluon condensate $\langle \alpha\,G^2 \rangle = 0.06 \pm 0.02 \ \mathrm{GeV}^4$. For the ground state, this correction amounts to the energy shift

$$\delta E_0 = \frac{624}{425} \, \frac{\pi \, \langle \alpha\,G^2 \rangle \, m}{(C_{\mathrm{F}}\,\tilde{\alpha}(\mu)\,m)^4} \ .$$

By inversion of the expression for the (ground-state) bound-state mass emerging from this procedure, the corresponding quark pole mass m is computed. For instance, with $\Lambda(n_{\mathrm{f}} = 4) = 0.23 \, ^{+0.08}_{-0.05}$ GeV and $\mu = \sqrt{6.632 \pm 25\,\%}$ GeV, implying $\alpha(\mu) = 0.246$ and $\tilde{\alpha}(\mu) = 0.386$, the experimental value [6] of the Υ mass, $M(\Upsilon)_{\mathrm{exp}} = 9.46037 \pm 0.00021$ GeV, translates into the b quark mass $m_{\mathrm{b}} = 5.001 \, ^{+0.104}_{-0.066}$ GeV [1].

However, a perturbative treatment as implied by the splitting (2) of the static potential $V_0^{\mathrm{P}}(r)$ is by no means mandatory, obligatory, or even desirable. We may also adopt the following point of view. Given the operator H defined by Eq. (1) (accurate up to a certain order in α), compute (numerically, if necessary) its discrete spectrum, i. e., the set of eigenvalues, irrespective of the involved powers of α. Of course, the terms in Eq. (1) proportional to

$$-\Delta^2 \ , \quad +\frac{1}{r}\,\Delta \ ,$$

and, if the effective coupling strength multiplying this term exceeds some critical value, also the term in Eq. (1) proportional to

$$-\frac{1}{r^2}$$

render the operator H unbounded from below and have therefore to be treated perturbatively anyway. The Hamiltonian

$$\hat{H} \equiv 2\,m - \frac{1}{m}\,\Delta + V_0^{\mathrm{P}}(r) \ , \tag{3}$$

on the other hand, may certainly be analyzed without adhering to some perturbative approximation.

In order to obtain a first idea of the differences brought about by these two approaches, let us start by considering only the Hamiltonian (3). The perturbative calculation is straightforward. Introducing, for notational brevity, the generalized Bohr radius

$$a(\mu) \equiv \frac{2}{C_{\rm F}\,\tilde{\alpha}(\mu)\,m}\ ,$$

the expectation values of the non-Coulombic interaction $\hat{V}(r)$ w. r. t. the ground state of $\tilde{H}$ (indicated by the subscript $\tilde{0}$) may be evaluated with the help of the relations (see also Appendix B of Ref. [4])

$$\begin{aligned}
\left\langle \frac{\ln(\mu\,r)}{r} \right\rangle_{\tilde{0}} &= \frac{1}{a(\mu)} \left[\ln\left(\frac{\mu\,a(\mu)}{2}\right) + 1 - \gamma_{\rm E} \right], \\
\left\langle \frac{\ln^2(\mu\,r)}{r} \right\rangle_{\tilde{0}} &= \frac{1}{a(\mu)} \left[\ln^2\left(\frac{\mu\,a(\mu)}{2}\right) + 2\,(1-\gamma_{\rm E})\,\ln\left(\frac{\mu\,a(\mu)}{2}\right) + (1-\gamma_{\rm E})^2 + \frac{\pi^2}{6} - 1 \right].
\end{aligned}$$

The nonperturbative evaluation of $\hat{H}$ is performed with some numerical procedure[1] developed for the treatment of the nonrelativistic Schrödinger equation [7]. In this way, we find, for the parameter values used in the second of Refs. [1] and focusing our interest to the ground state, for the Coulomb binding energy, $\varepsilon_0 = -0.33146$ GeV, for the expectation value of $\hat{V}(r)$, $\langle \hat{V}(r) \rangle_{\tilde{0}} = -0.13714$ GeV, and thus, for the perturbatively calculated ground-state energy,[2] $\hat{E}_0^{\rm P} \equiv 2\,m + \varepsilon_0 + \langle \hat{V}(r) \rangle_{\tilde{0}} = 9.5334$ GeV, while the numerically computed "exact" lowest eigenvalue of the operator (3) is $\hat{E}_0^{\rm NP} \equiv \langle \hat{H} \rangle_0 = 9.5198$ GeV. Consequently, for the parameters of Ref. [1] the difference in the lowest bound-state mass predicted by the Hamiltonian (3) within perturbative and nonperturbative approaches is $\hat{E}_0^{\rm P} - \hat{E}_0^{\rm NP} = 13.6$ MeV. Unfortunately, this discrepancy is roughly 65 times larger than the experimental error on the Υ mass. Phrased the other way round, the perturbative ground-state eigenvalue $\hat{E}_0^{\rm P}$ of $\hat{H}$ can be reproduced by the nonperturbative evaluation of $\hat{H}$ for a mass m of the bound-state constituents of $m = 5.008$ GeV. For the b quark mass of Ref. [1], the theoretical error different from the one induced by variation of the renormalization scale μ, attributed to neglected higher-order perturbative as well as nonperturbative corrections, is estimated to be ± 0.006 GeV. Obviously, this error is entirely consumed already by the difference of the masses of the bound-state constituents obtained by perturbative and nonperturbative evaluations of $\hat{H}$.

In view of these findings, let's try to improve the theoretical value of the b quark pole mass $m_{\rm b}$ by approaching the part $\hat{H}$ of the Hamiltonian (1) nonperturbatively. The numerical computation of the expectation values of the operator $H - \hat{H}$ is considerably facilitated by the following two observations:

- The eigenvalue equation for the "toy-model" (Hamiltonian) operator $\hat{H}$ defined in Eq. (3) reads, for some generic (energy) eigenvalue $\hat{E}$ and its corresponding eigenstate $|\psi\rangle$ of $\hat{H}$, $\hat{H}|\psi\rangle = \hat{E}\,|\psi\rangle$. Thus the expectation values of all terms in the Hamiltonian (1) involving the Laplacian Δ, taken w. r. t. $|\psi\rangle$, may be evaluated by substituting Δ according to $\Delta|\psi\rangle = m\left[2\,m + V_0^{\rm P}(r) - \hat{E}\right]|\psi\rangle$.

- The expectation value of the δ function entering in the "spin–spin term" of the Hamiltonian (1), taken w. r. t. $|\psi\rangle$, is the modulus squared of the corresponding wave function $\psi(\mathbf{x})$ at the origin: $\langle\psi|\delta^{(3)}(\mathbf{x})|\psi\rangle = |\psi(\mathbf{0})|^2$. For states with vanishing orbital angular momentum ℓ (the so-called "S waves"), $|\psi(\mathbf{0})|^2$ may be expressed in terms of the first derivative of the relevant interaction potential $V(r)$ w. r. t. the radial coordinate r according to (for a derivation, see, e. g., Ref. [8])

$$|\psi(\mathbf{0})|^2 = \frac{m}{4\,\pi} \left\langle \psi \left| \frac{\rm d}{{\rm d}r} V(r) \right| \psi \right\rangle .$$

In this way, the lowest eigenvalue of the Hamiltonian H may be computed from the expression (where the subscript 0 of the expectation values indicates, as before, the ground state of the Hamiltonian $\hat{H}$)

$$\begin{aligned}
E_0 \equiv \langle H \rangle_0 &= \hat{E}_0^{\rm NP} - \frac{1}{4\,m^3} \left\langle \Delta^2 \right\rangle_0 + \frac{C_{\rm F}\,\alpha(\mu)}{m^2} \left\langle \frac{1}{r}\,\Delta \right\rangle_0 + \frac{C_{\rm F}\,\alpha^2(\mu)}{4\,m}\,(C_{\rm F} - 2\,C_{\rm A}) \left\langle \frac{1}{r^2} \right\rangle_0 \\
&+ \frac{4\,\pi\,C_{\rm F}\,\alpha(\mu)}{3\,m^2}\,s\,(s+1)\,|\psi_0(\mathbf{0})|^2\ .
\end{aligned}$$

[1] The desired accuracy of the (numerically determined) bound-state energies and wave functions may be adjusted in the routine used for the solution of the Schrödinger equation. For the present analysis, the uncertainty of these energies has been required to be less than 10^{-7} GeV = 100 eV. This accuracy should be, by far, sufficient for our purposes.

[2] For the perturbative treatment of $\hat{H}$, we truncate the Rayleigh–Schrödinger series for $\hat{E}_0^{\rm P}$ at lowest non-trivial order in $\hat{V}(r)$. Inclusion of the next order [1] reduces the observed discrepancies but does not change qualitatively our findings.

Adding the nonperturbative shift δE_0 gives our final result for the ground-state energy: $\mathcal{E}_0 = E_0 + \delta E_0$. For the parameter values of Ref. [1] and a b quark mass of $m_{\rm b} = 5.001$ GeV, this expression entails the bound-state energy $\mathcal{E}_0 = 9.4953$ GeV. Hence, the error of the predicted Υ mass brought about by the perturbative approximation in the treatment of the Hamiltonian (1), which amounts to 35 MeV, is of the order of the hyperfine splittings in the bottomonium system. For the latter, the second of Refs. [1] quotes, e. g., $M(\Upsilon) - M(\eta_{\rm b}) = 46.6\,^{+14.8}_{-12.7}$ MeV.

Consequently, a re-evaluation of the b quark mass appears to be in order. Fitting the ground-state bound-state energy $\mathcal{E}_0$, for the numerical values of the parameters Λ, μ, and $\langle \alpha\, G^2 \rangle$ adopted in Ref. [1], to the experimental mass of the Υ, we obtain for the pole mass of the b quark

$$m_{\rm b} = 4.983 \text{ GeV} \; .$$

The errors caused by the uncertainties of Λ and $\langle \alpha\, G^2 \rangle$ and by the variation of μ should be practically the same as in Ref. [1]. Hence, dropping the requirement of analytical accessibility of the Hamiltonian (1) reduces the extracted b quark mass by some 18 MeV. A very similar result is expected to be found for the determination of the c quark mass. We arrive at the conclusion that in Refs. [1] the theoretical errors on the quark masses have been somewhat underestimated.

Note that the above considerations apply, of course, also to the analysis presented in Ref. [4]. Note also that the correct [3] numerical factor in the numerator of the first term in the expression for the three-loop β function coefficient β_2 differs slightly from the one used in Refs. [1].

References

[1] A. Pineda and F. J. Ynduráin, Phys. Rev. D **58** (1998) 094022; hep-ph/9812371.

[2] M. Peter, Phys. Rev. Lett. **78** (1997) 602; Nucl. Phys. B **501** (1997) 471;
Y. Schröder, Phys. Lett. B **447** (1999) 321; hep-ph/9909520.

[3] O. V. Tarasov, A. A. Vladimirov, and A. Yu. Zharkov, Phys. Lett. B **93** (1980) 429.

[4] S. Titard and F. J. Ynduráin, Phys. Rev. D **49** (1994) 6007.

[5] M. B. Voloshin, Nucl. Phys. B **154** (1979) 365;
H. Leutwyler, Phys. Lett. B **98** (1981) 447.

[6] C. Caso *et al.* (Particle Data Group), Eur. Phys. J. C **3** (1998) 1.

[7] W. Lucha and F. F. Schöberl, Int. J. Mod. Phys. C **10** (1999) 607, hep-ph/9811453.

[8] W. Lucha, F. F. Schöberl, and D. Gromes, Phys. Rep. **200** (1991) 127.